

A Scalable Optimization Approach for the Multilinear System Arising from Scattered Data Interpolation

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Abstract. Scattered data interpolation aims to reconstruct a continuous (smooth) function that approximates the underlying function by fitting (meshless) data points. There are extensive applications of scattered data interpolation in computer graphics, fluid dynamics, inverse kinematics, machine learning, etc. In this paper, we consider a novel generalized Mercer kernel in the reproducing kernel Banach space for scattered data interpolation. The system of interpolation equations is formulated as a multilinear system with a structural tensor, which is an absolutely and uniformly convergent infinite series of symmetric rank-one tensors. Then we design a fast numerical method for computing the product of the structural tensor and any vector in arbitrary precision. Whereafter, a scalable optimization approach equipped with limited-memory BFGS and Wolfe line-search techniques is customized for solving these multilinear systems. Using the Łojasiewicz inequality, we prove that the proposed scalable optimization approach is a globally convergent algorithm and possesses a linear or sublinear convergence rate. Numerical experiments illustrate that the proposed scalable optimization approach can improve the accuracy of interpolation fitting and computational efficiency.

AMS subject classifications: 15A69, 65H10, 90C30, 90C90

Key words: Scattered data interpolation, generalized Mercer kernel, structural tensor, multilinear system, optimization, Łojasiewicz inequality.

1 Introduction

Scattered data consists of a set of data sites $X := \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \Omega$ and corresponding values $V := \{f_1, \dots, f_N\} \subset \mathbb{R}$, where $\Omega \subseteq \mathbb{R}^d$ is locally compact. Here, “scattered” means that

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the data sites have no structure or order between their relative locations. The values come from an underlying (not necessarily known) function. Scattered data interpolation aims to reconstruct a (typically smooth) function $s(\mathbf{x})$ that approximates the underlying function and particularly satisfies

$$s(\mathbf{x}_i) = f_i, \quad \forall i = 1, \dots, N. \quad (1.1)$$

Scattered data interpolation has extensive applications in computer graphics [2], fluid dynamics [14], inverse kinematics [17], machine learning [37], etc. When data sites enjoy a well mesh geometry, plenty of methods such as wavelets, multivariate splines, and finite elements have been used for the interpolation problem (1.1). However, in the context of scattered data interpolation, meshless methods including radial basis functions [9] and kernel-based approximations [37] are promising. The monograph [41] provides more details. We focus on kernel-based methods in this paper.

To separate the influence between data sites and values, functions $u_j : \mathbb{R}^d \rightarrow \mathbb{R}$ ($j = 1, \dots, N$) that depend only on \mathbf{x} are chosen to form

$$s(\mathbf{x}) = \sum_{j=1}^N f_j u_j(\mathbf{x}).$$

We note that the Lagrange interpolation is equipped with $u_j(\mathbf{x}_i) = \delta_{ij}$ for $i, j \in \{1, \dots, N\}$, where δ_{ij} stands for the Kronecker delta. However, due to the Mairhuber-Curtis theorem [41, Theorem 2.3], continuous functions $\{u_j\}$ satisfying $u_j(\mathbf{x}_i) = \delta_{ij}$ may not always exist and be unique when $d \geq 2$.

Kernel methods [37] are a class of simple and powerful approaches for solving the interpolation problem (1.1). The reproducing kernel Hilbert space (RKHS) provides a reproducing kernel $K : \Omega \times \Omega \rightarrow \mathbb{R}$ and the associated interpolation function is defined as

$$s(\mathbf{x}) = \sum_{j=1}^N c_j K(\mathbf{x}, \mathbf{x}_j), \quad (1.2)$$

where c_j for $j = 1, \dots, N$ are undetermined real coefficients. The kernel K ensures that matrix $A := [K(\mathbf{x}_i, \mathbf{x}_j)] \in \mathbb{R}^{N \times N}$ is positive definite or conditionally positive definite for any set $X \subset \Omega$ of data sites [41]. Fasshauer and Ye [16] gave a unified theory for conditionally positive definite kernels. Combining the interpolation condition (1.1) and the interpolation function (1.2), we get the following linear system:

$$A\mathbf{c} = \mathbf{b}, \quad (1.3)$$

where $\mathbf{c} := (c_1, \dots, c_N)^\top$ is an undetermined vector and $\mathbf{b} := (f_1, \dots, f_N)^\top$ is the value vector. By solving the linear system (1.3), we determine coefficients in (1.2) and hence obtain the interpolation function $s(\mathbf{x})$.

Using the novel generalized Mercel kernel in the reproducing kernel Banach space (RKBS) [15], Xu and Ye [43] proposed the following system of polynomial equations for